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Study of θ dependence in Yang-Mills theories on the lattice

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We discuss the use of field theoretical techniques in the lattice determination of the free energy dependence on the θ angle in SU(N) Yang-Mills theories.

1 Introduction

The dependence of the free energy density $F(\theta)$ of Yang-Mills theories on the θ angle is the subject of ongoing theretical debate. $F(\theta)$ is defined as:

$$\exp[-VF(\theta)] \equiv \int [dA]\, e^{-\int d^4x \mathcal{L}(x)}\, e^{i\theta Q} \tag{1}$$

where $\mathcal{L}(x) = \frac{1}{4} F^a_{\mu\nu}(x) F^a_{\mu\nu}(x)$ is the usual Yang Mills lagrangian and $Q = \int \mathrm{d}^4x\ q(x)$ is the topological charge, with the topological charge density $q(x)$ defined as

$$q(x) = \frac{g^2}{64\pi^2} \epsilon_{\mu\nu\rho\sigma} F^a_{\mu\nu}(x) F^a_{\rho\sigma}(x) = \partial_\mu K_\mu(x) \,, \tag{2}$$

where $K_\mu(x)$ is the Chern current

$$K_\mu = \frac{g^2}{16\pi^2} \epsilon_{\mu\nu\rho\sigma} A^a_\nu \left(\partial_\rho A^a_\sigma - \frac{1}{3} g f^{abc} A^b_\rho A^c_\sigma \right) \tag{3}$$

The determination of $F(\theta)$ is a typical non-perturbative problem and lattice QCD is in principle a natural tool to deal with it, but the complex nature of the euclidean action for $\theta \neq 0$ forbids the use of standard Monte Carlo simulations. However many interesting physical aspects can be analyzed by studying $F(\theta)$ for small values of θ. The terms in the Taylor expansion of $F(\theta)$ around $\theta = 0$

$$F(\theta) = F(0) + \sum_{k=1}^{\infty} \frac{1}{k!} F^{(k)}(0) \theta^k \tag{4}$$

are related to the connected moments of the topological charge distribution at $\theta = 0$:

$$F^{(k)}(0) \equiv \frac{d^k}{d\theta^k} F(\theta)|_{\theta=0} = -i^k \frac{\langle Q^k \rangle_c}{V} \,, \tag{5}$$

which can be determined by standard lattice Monte Carlo simulations[1].

[1]Other approaches for a determination of $F(\theta)$ have been tried, based on a Fourier transform of the topological charge distribution or on extrapolations from simulations at imaginary values of θ [1]

The quadratic term is proportional to the topological susceptibility, $\chi = \langle Q^2 \rangle / V$, which is expected to be $\neq 0$ to the leading order in $1/N_c$ in order to solve the so-called $U(1)$ problem [2, 3]. It has been already extensively studied by lattice simulations (see Refs. [4, 5] for recent reviews): since the study of topological quantities on the lattice is always non-trivial, several methods have been used: cooling, the field theoretical method, and fermionic methods based on the index theorem, all giving consistent results for χ and in agreement with the Witten-Veneziano formula relating χ to the η' mass.

It has been argued that, for $\theta < \pi$, $F(\theta)$ is almost quadratic in θ, with $O(\theta^4)$ corrections suppressed by powers of $1/N_c$ [6, 7]. In order to verify this conjecture it is interesting to obtain a lattice determination of the quartic term in the expansion of $F(\theta)$ and measure its relative weight with respect to the quadratic one. This has been done using the cooling method [8] and the field theoretical methd [9]. In the following I will illustrate the details of the lattice determination in the framework of the field theoretical method and compare the results with those obtained by the cooling method. Further details can be found in Ref. [9].

2 The method

On the lattice it is possible to define a discretized gauge invariant topological charge density operator $q_L(x)$, and a related topological charge $Q_L = \sum_x q_L(x)$ (with the sum extended over all lattice points), with the only requirement that, in the formal (naïve) continuum limit,

$$q_L(x) \stackrel{a \to 0}{\sim} a^4 q(x) + O(a^6) \,, \tag{6}$$

where a is the lattice spacing. A possible definition is

$$q_L(x) = \frac{-1}{2^9 \pi^2} \sum_{\mu\nu\rho\sigma=\pm 1}^{\pm 4} \tilde{\epsilon}_{\mu\nu\rho\sigma} \mathrm{Tr} \left(\Pi_{\mu\nu}(x) \Pi_{\rho\sigma}(x) \right) \,, \tag{7}$$

where $\Pi_{\mu\nu}(x)$ is the usual plaquette operator in the $\mu\nu$ plane, $\tilde{\epsilon}_{\mu\nu\rho\sigma}$ is the standard Levi–Civita tensor for positive directions and is otherwise defined by the rule $\tilde{\epsilon}_{\mu\nu\rho\sigma} = -\tilde{\epsilon}_{(-\mu)\nu\rho\sigma}$.

A proper renormalization must be performed when going towards the continuum limit, like for any other regularized operator. For instance, in spite of the formal limit in Eq. (6), the discretized topological charge density renormalizes multiplicatively [10]:

$$q_L(x) = Z(\beta)a^4(\beta)q(x) + O(a^6) \ , \tag{8}$$

with a multiplicative renormalization constant $Z(\beta)$ which is a finite function of the bare coupling $\beta = 2N/g_0^2$, approaching 1 as $\beta \to \infty$.

Further renormalization constants, relating lattice to continuum quantities, may appear when defining correlation functions of the topological charge. For example, in the case of the topological susceptibility,

$$\chi \equiv \frac{\langle Q^2\rangle}{V} = \int \mathrm{d}^4x \ \langle q(x)q(0)\rangle \ , \tag{9}$$

one in general is not guaranteed that the lattice definition

$$\chi_L = \sum_x \langle q_L(x)q_L(0)\rangle \tag{10}$$

satisfy the correct continuum prescription for the contact term arising in Eq. (9) as $x \to 0$, and this leads to the appearance of an additive renormalization, so that the lattice quantity χ_L is related to the continuum quantity χ by

$$\chi_L = Z(\beta)^2 a^4(\beta)\chi + M(\beta) \ . \tag{11}$$

The idea of the field theoretical method for the determination of χ is to compute and then subtract the renormalization constants from the lattice quantity χ_L, following Eq. (11). The determination can be performed numerically using the so–called *heating method* [10, 11, 12, 13, 14, 15, 16, 17, 18]: the renormalization constants are related to the UV fluctuations living on the scale of the lattice spacing that, close enough to the continuum limit, are effectively decoupled from the topological modes living on physical scales. It is thus possible to create samples of configurations of fixed topological background with the UV fluctuations thermalized, by heating a semiclassical configuration of initial charge Q. Expectation values on this samples give the necessary information:

$$\begin{aligned}\langle Q_L\rangle &= Z(\beta)\ Q \\ \langle Q_L^2\rangle &= Z(\beta)\ Q^2 + V\ M(\beta)\end{aligned} \tag{12}$$

(this is also, in some sense, the idea at the basis of cooling, in which the UV fluctuations are suppressed by a process of local minimization of the action, without hopefully altering the background topological content, in order to remove the renormalizations, i.e. $Z \to 1$ and $M \to 0$).

Improved (smeared) operators [19] can be used in order to reduce the renormalization effects, thus leading to improved estimates of χ.

Let us now turn to the problem of the determination of the connected quartic moment, $\langle Q^4\rangle_c = \langle Q^4\rangle - 3\langle Q^2\rangle^2$. It is clearly necessary to first understand how the lattice expectation value $\langle Q_L^4\rangle$ renormalizes with respect to the continuum $\langle Q^4\rangle$. Apart from an obvious $Z(\beta)$ multiplicative renormalization, there will be additive renormalizations coming from contact terms appearing in

$$\langle Q_L^4\rangle = \int \mathrm{d}^4x_1 \ldots \mathrm{d}^4x_4 \langle q_L(x_1)\ldots q_L(x_4)\rangle \tag{13}$$

as two or more charge densities come to the same point ($x_i \sim x_j$ for some i, j).

It can be shown [9] that a quite natural assumption for the renormalization rule is the following

$$\langle Q_L^4\rangle = Z(\beta)^4\langle Q^4\rangle + M_{4,2}(\beta)\langle Q^2\rangle + M_{4,0}(\beta) \tag{14}$$

This assumption can be shown to be theoretically sensible and allows a straightforward extension of the heating method to determine the two new renormalization constants $M_{4,2}(\beta)$ and $M_{4,0}(\beta)$.

Indeed, the measurement of $\langle Q_L^4\rangle$ on a sample of configurations with background topological charge Q gives

$$\langle Q_L^4\rangle = Z^4(\beta)\ Q^4 + M_{4,2}(\beta)\ Q^2 + M_{4,0}(\beta) \tag{15}$$

and if the measurement is repeated in at least two different topological sectors, sufficient constraints are obtained to determine $M_{4,2}(\beta)$ and $M_{4,0}(\beta)$. If more topological sectors are used, there is an excess of constraints which can be exploited as a non-trivial test of the method.

In the general case of the n-th order correlation function, a natural extension of Eq. (14) is the following:

$$\langle Q_L^n\rangle = Z^n\langle Q^n\rangle + \sum_{h=1}^{n/2} M_{n,n-2h}\langle Q^{n-2h}\rangle \ , \tag{16}$$

and its validity can be discussed along the same lines as for $n = 4$ [9].

3 Results

The method has been applied to the case of $SU(3)$ pure gauge theory, on a 16^4 lattice at $\beta = 6.1$, using 1–smeared and 2–smeared operators [19, 16].

We have collected five different samples of configurations, one thermalized in the $Q = 0$ sector (around the zero field configuration), two in the $Q = 1$ sector (thermalized around two different semiclassical configurations of topological charge one) and two in the $Q = 2$ sector (thermalized around two different semiclassical configurations of topological charge two). The semiclassical configurations have been obtained by extracting thermalized configurations with non-trivial topology from the equilibrium ensemble at $\beta = 6.1$ and then minimizing their action by a usual cooling technique. All the five samples have been obtained by performing about 3000 heating trajectories around the semiclassical configurations, each trajectory consisting of 90 heating steps; 6 straight cooling steps have been applied on heated configurations to check that their background topological content did not change.

We have then measured the expectation values $\langle Q_L^2\rangle$, $\langle Q_L^4\rangle$, and also $\langle Q_L\rangle/Q$ where $Q \neq 0$, over the five samples. We have reported the results in Table 1 for the 1-smeared operator and in Table 2 for the 2-smeared operator: expectation values obtained on samples with the same Q turned out to be equal within errors, as they should, and we have reported in the tables only their weighted averages. Those data have then been used to perform a fit to Eqs. (12) and (15) obtaining finally the values of the renormalization constants reported in Table 3.

Table 1. Expectation values measured in different topological sectors for the 1-smeared operator.

Q	$Z = \langle Q_L\rangle/Q$	$\langle Q_L^2\rangle$	$\langle Q_L^4\rangle$
0	-	0.311(12)	0.290(20)
1	0.416(6)	0.4785(60)	0.630(15)
2	0.413(5)	0.9626(80)	1.973(50)

Table 2. Expectation values measured in different topological sectors for the 2-smeared operator.

Q	$Z = \langle Q_L\rangle/Q$	$\langle Q_L^2\rangle$	$\langle Q_L^4\rangle$
0	-	0.208(10)	0.124(10)
1	0.544(5)	0.489(5)	0.556(12)
2	0.542(4)	1.314(8)	2.77(6)

The equilibrium values $\langle Q_L^2\rangle$ and $\langle Q_L^4\rangle$, which are reported in Table 4, have been measured on a sample of 300K configurations separated by five updating cycles, each composed of a mixture of 4 over-relaxation + 1 heat-bath updating sweeps; the reported errors have been estimated by a standard blocking technique.

Using Eqs. (11) and (14) we can compute $\langle Q^2\rangle$ and $\langle Q^4\rangle$, obtaining the results reported in Table 4. It is interesting to notice that the values obtained for the 1-smeared operator and for the 2-smeared operator are in good agreement, as they should, confirming the correctness of the method.

We can finally determine $\langle Q^4\rangle_c = \langle Q^4\rangle - 3\langle Q^2\rangle^2$, obtaining $\langle Q^4\rangle_c = 0.32 \pm 1.80$ for the 1-smeared and $\langle Q^4\rangle_c = 0.66 \pm 0.90$ for the 2-smeared operator, leading to $b_2 = -0.012(62)$ and $b_2 = -0.024(32)$ for the 1-smeared and 2-smeared operator respectively, in agreement with the determination reported in Ref. [8].

Table 3. Values of the renormalization constants obtained respectively for the 1-smeared and 2-smeared operators, by using the results reported in tables 1 and 2 and performing a best fit to Eqs. (12) and (15).

Z	VM	$M_{4,0}$	$M_{4,2}$
0.414(4)	0.315(6)	0.336(16)	0.289(16)
0.543(5)	0.211(5)	0.377(15)	0.124(9)

Table 4. Expectation values measured at equilibrium and results obtained for the renormalized quantities, respectively for the 1-smeared and 2-smeared operators.

$\langle Q_L^2\rangle$	$\langle Q_L^4\rangle$	$\langle Q^2\rangle$	$\langle Q^4\rangle$
0.7121(38)	1.548(18)	2.312(72)	16.4 ± 1.8
0.8776(60)	2.368(36)	2.262(41)	16.02(72)

4 More on the renormalization effects

The renormalization constants Z, $M_{n,m}$ ($m < n$) which, for a given lattice discretization Q_L, appear in Eq. (16), are in principle independent of each other, or at least no simple relation exists among them, unless some further hypothesis can be done about the nature of the UV fluctuations which are responsible for the renormalizations. We will propose and test an ansatz which will greatly simplify the structure of the renormalization constants and will lead to a renormalization formula which directly involves the connected correlation functions, thus allowing a more precise determination of b_2.

An hypothesis about the nature of the UV fluctuations has been done in Refs. [11, 13], where it was assumed that the discretized topological charge density can be expressed as

$$q_L(x) \simeq [Z + \zeta(x)]q(x) + \eta(x) \;, \tag{17}$$

where $q(x)$ is a background topological charge density which is determined by physical fluctuations on the scale of the correlation length ξ, whereas $\zeta(x)$ and $\eta(x)$ are random variables with zero averages which are determined by the short range UV fluctuations and, at least in the continuum limit, are expected to be decoupled from $q(x)$, i.e. $\langle\zeta(x)q(x)\rangle = \langle\eta(x)q(x)\rangle = 0$. Summing Eq. (17) over all lattice points, the following relation follows for the lattice topological charge Q_L:

$$Q_L = Z\; Q + \sum_x \zeta(x)q(x) + \eta \;, \tag{18}$$

where $\eta = \sum_x \eta(x)$. We now make the further assumption that the term $\sum_x \zeta(x)q(x)$ in Eq. (18) can be neglected, configuration by configuration. This is not unreasonable, in view of the fact that $q(x)$ and $\zeta(x)$ are decoupled from each other. We will thus assume that

$$Q_L = Z\; Q + \eta \;, \tag{19}$$

where η is a random noise with zero average which is stochastically independent of Q.

This assumption has relevant consequences for the structure of the renormalization constants. Indeed, using the hypothesis that Q and η are stochastically independent variables and that they are both evenly distributed around zero, it is easy to verify that the general renormalization formula holds:

$$\langle Q_L^n\rangle = \sum_{h=0}^{n/2} \binom{n}{2h} Z^{n-2h}\langle Q^{n-2h}\rangle\langle\eta^{2h}\rangle \;, \tag{20}$$

so that the renormalization relation for $\langle Q_L^n\rangle$ is described only in terms of Z and of the correlation functions of the noise η. In particular we have $M_{n,m} = \binom{n}{m} Z^m\langle\eta^{n-m}\rangle$, a relation that should be verified on numerical data if our ansatz in Eq. (19) is correct. From the data in Table 3 it can be checked that indeed $M_{4,2} = 6Z^2\langle\eta^2\rangle = 6Z^2VM$, but we will now proceed further and check the validity of Eq. (20) up to $n = 6$. The correlation functions of η can be determined by the heating method using the analogous of Eq. (15), which up to $n = 6$ reads:

$$\begin{aligned}
\langle Q_L^2\rangle &= Z^2Q^2 + \langle\eta^2\rangle \\
\langle Q_L^4\rangle &= Z^4Q^4 + 6Z^2Q^2\langle\eta^2\rangle + \langle\eta^4\rangle \\
\langle Q_L^6\rangle &= Z^6Q^6 + 15Z^4Q^4\langle\eta^2\rangle + \\
&\quad +15Z^2Q^2\langle\eta^4\rangle + \langle\eta^6\rangle \;.
\end{aligned} \tag{21}$$

Using the values for $\langle Q_L^2\rangle$, $\langle Q_L^4\rangle$ and $\langle Q_L^6\rangle$ obtained in the sectors with $Q = 0, 1, 2$ we have performed a best fit to Eqs. (21), obtaining the best fit values reported in Table 5 with $\chi^2/\text{d.o.f.} \simeq 0.34$ for the 1-smeared operator and $\chi^2/\text{d.o.f.} \simeq 0.23$ for 2-smeared operator. The fact that the values for $\langle Q_L^2\rangle$, $\langle Q_L^4\rangle$ and $\langle Q_L^6\rangle$ obtained in the various sectors can be fitted by the simple relations in Eq. (21) is a confirmation of the validity of the ansatz in Eq. (19).

Assuming that Eq. (19) is valid, it is possible to write a renormalization relation which involves directly the connected correlation functions. Indeed, it is a general rule that the connected correlation functions of a stochastic variable (Q_L in our case), which is the sum of two variables which are stochastically independent of each other (ZQ and η in our case), are the sum of the corresponding connected correlation functions, i.e.

$$\langle Q_L^n\rangle_c = Z^n\langle Q^n\rangle_c + \langle\eta^n\rangle_c \;. \tag{22}$$

Therefore in order to compute $\langle Q^n\rangle_c$ we need to know, apart from Z, only one renormalization constant, $\langle\eta^n\rangle_c$, which can be easily measured by computing $\langle Q_L^n\rangle_c$ on the sample of configurations in the $Q = 0$ sector. $\langle Q^n\rangle_c$ is then given by

$$\langle Q^n\rangle_c = \frac{\langle Q_L^n\rangle_c - \langle\eta^n\rangle_c}{Z^n} \;, \tag{23}$$

where $\langle Q_L^n\rangle_c$ is measured on the ensemble of configurations at equilibrium.

We have computed $\langle Q_L^4\rangle_c = \langle Q_L^4\rangle - 3\langle Q_L^2\rangle^2$ on our equilibrium configurations at $\beta = 6.1$, obtaining $\langle Q_L^4\rangle_c = 0.026(7)$ for the 1-smeared operator and $\langle Q_L^4\rangle_c = 0.057(13)$ for the 2-smeared operator. We have then computed $\langle Q_L^4\rangle_c$ on our sample of configurations thermalized in the $Q = 0$ sector at $\beta = 6.1$, obtaining $\langle\eta^4\rangle_c = \langle\eta^4\rangle - 3\langle\eta^2\rangle^2 = 0.006(4)$ for the 1-smeared operator and $\langle\eta^4\rangle_c = 0.001(2)$ for the 2-smeared operator. In both cases (equilibrium and $Q = 0$) errors have been estimated by standard jackknife techniques.

By using Eq. (23) and the values for Z and $\langle Q^2\rangle$ previously obtained, we have obtained $\langle Q^4\rangle_c = 0.68(24)$, $b_2 = -0.024(9)$ for the 1-smeared operator and $\langle Q^4\rangle_c = 0.66(15)$, $b_2 = -0.024(6)$ for the 2-smeared operator.

By making use of the ansatz in Eq. (19) we have thus made determinations which are much more precise than those obtained in Section 3. The reason is that Eq. (22) allows to relate $\langle Q^n\rangle_c$ directly to the connected correlation functions of the discretized lattice topological charge, with only two renormalization constants involved: this greatly simplifies computations and error propagation, thus leading to improved estimates. We notice that most of the error in the final determination of $\langle Q^4\rangle_c$ and b_2 comes from the determination of $\langle Q_L^4\rangle_c$ at equilibrium, which is also the most expensive part of the computation in terms of CPU time.

The renormalization procedure is thus completely under control and numerically non expensive.

We have also made a determination of b_2 at $\beta = 6.0$, again on a 16^4 lattice. On a sample of about 300K configurations obtained at equilibrium and using the same algorithm as for $\beta = 6.1$ we have obtained, for the 2-smeared operator, $\langle Q_L^2 \rangle = 1.377(7)$, $\langle Q_L^4 \rangle_c = 0.052(23)$. On a sample of configurations thermalized in the $Q = 0$ topological sector by performing about 3000 heating trajectories, each composed of 90 heating steps, we have obtained, for the 2-smeared operator, $\langle \eta^2 \rangle = 0.308(10)$ and $\langle \eta^4 \rangle_c = 0.002(3)$. From these data, using the value $Z(\beta = 6.0) = 0.51(2)$ reported for the 2-smeared operator in Ref. [16], we obtain $b_2 = -0.015(8)$, which is consistent with the value obtained at $\beta = 6.1$.

Let us close noticing that the value obtained for $\langle \eta^4 \rangle_c$ is very small and compatible with zero for both the 1-smeared and the 2-smeared operator. We have also measured $\langle \eta^6 \rangle_c$ on the sample of configurations at $Q = 0$ obtaining $\langle \eta^6 \rangle_c = 0.001(8)$ for the 1-smeared and $\langle \eta^6 \rangle_c = 0.0005(14)$ for 2-smeared operator ($\beta = 6.1$), so that η behaves with a good approximation as a pure gaussian noise.

Table 5. Values of the renormalization constants, respectively for the 1-smeared and 2-smeared operators, obtained by performing a best fit to Eq. (21).

Z	$\langle \eta^2 \rangle$	$\langle \eta^4 \rangle$	$\langle \eta^6 \rangle$
0.415(4)	0.315(6)	0.298(11)	0.462(37)
0.542(4)	0.211(5)	0.129(6)	0.131(17)

5 Conclusions

We have discussed the extension of the field theoretical method, already used for the lattice determination of the topological susceptibility, to the computation of further terms in the expansion of the ground state energy $F(\theta)$ around $\theta = 0$.

We have presented numerical results regarding SU(3) pure gauge theory, providing a determination of the fourth order term in the expansion of $F(\theta)$ around $\theta = 0$. Our determination is in agreement with that obtained in Ref. [8] via the cooling method, and confirms that fourth order corrections to the simple θ^2 behaviour of $F(\theta)$ around $\theta = 0$ are small already for $N_c = 3$.

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